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M. Ilias

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THE ALL-ELECTRON TREATING OF THE SPIN-ORBIT INTERACTION BASED ON SINGLE-DETERMINANT WAVEFUNCTION

MIROSLAV ILIAS

Department of Physical Chemistry, Faculty of Natural Sciences,
Comenius University Bratislava, Mlynska dolina CH-1, SK-84215 Bratislava, Slovakia
E-mail: ilias@fns.uniba.sk

Two possible approaches for treating the spin-orbit effects in heavy element systems are presented here: a) The double-perturbative treatment at the post-HF level together with the electron correlation, b) The variational two-component approach where the spin-orbit term is added to the scalar Hamiltonian and the energy functional is minimized. The former is proposed for calculating the spin-orbit energy shift in closed-shell systems, the latter is suitable also for calculating the spin-orbit splitting in open-shell systems. In both approaches the effective one-electron (mean-field) spin-orbit operator is used.